

Piperazine
110-85-0 | DTXSID1021164

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.39e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.85e-01

Confidence level: 7.47e-01

Nearest Neighbors from the Training Set

Image not found

1-Butanethiol

Measured: 5.10e-11

Predicted: 3.36e-11

Image not found

1,4-Diazabicyclo[2.2.2]octane

Measured: 2.20e-11

Predicted: 1.30e-11

Image not found

1-Butanol

Measured: 8.57e-12

Predicted: 1.06e-11

Image not found

2-Butanol

Measured: 9.60e-12

Predicted: 8.64e-12

Image not found

1-Propanol

Measured: 5.53e-12

Predicted: 7.35e-12